Supplementary Data:

Table 1*: Binding Energy profiles (KcalMOl-1) of the five experimental phytosterols with Estrogen Receptor Alpha (ERα), 1X7R.*

Compounds	Total Binding Energy	Hydrogen Bonding Pattern			Other weakly interacting residues
		H-bonds	Bond Energy	Bond Length (Å)	
β-sitosterol	-0.3871	O PRO-324-A-H67	-4.7	1.91	Arg394, Trp393, Ile326, Glu323
Stigmasterol	-1.7866	H LEU-462-A-O25 OG SER-468-A-H65	-4.7 -4.7	1.86 2.05	His373, Thr371, Lys467, Leu462, Thr465, Ser468, Asp374
α-Spinasterol	-1.3504	O PRO-324-A-H65	-4.7	1.92	Glu323, Trp393
Campesterol	-1.3493	H LEU-462-A-O27 OG SER-468-A-H71	-4.7 -4.7	1.86 2.05	Thr371, Lys467, His373, Thr465, Ser468, Leu462, Asp374
Ergosterol	-4.7943	HZ_1 LYS-449-A-O27	-4.7	1.80	Arg394, Glu323, Trp393, Ile326, Pro324, Phe445, Gly390

Table 2*: Details of the 50 known inhibitors of Er-α subtype and their corresponding inhibitory concentrations (IC50) values used to generate the 2D-QSAR model.*

BindingDB_id	Ligand SMILES	IC_{50} (nM)
50973510	Oc1ccc(cc1)-c1sc2cccc(O)c2c1C(=O)c1ccc(OCCN2CCCCC2)cc1	0.002
714547	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)CO)c1c(F)ccc(OCCNCCCF)c1C	0.034
714621	COc1ccc(OCCNCCCF)c(F)c1[C@H]1N(CC(F)F)[C@H](C)Cc2c1[nH]c1ccccc21	0.042
714677	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)CO)c1c(F)cnc(OCCNCCCF)c1C	0.045
50973669	Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)-c1ccc(Cl)cc1	0.046
575938	C[C@@H]1Cc2c(ccc3[nH]nc(F)c23)[C@H](N1CC(F)(F)F)c1ccc(NC2CN(CCCF)C2)c(F)n1	0.048
575914	C[C@@H]1Cc2c(ccc3[nH]ncc23)[C@H](N1CC(F)(F)F)c1ccc(NC2CN(CCCF)C2)cc1	0.05
575876	C[C@@H]1Cc2c(ccc3[nH]ncc23)[C@H](N1CC(F)(F)F)c1c(F)cc(NC2CN(CCCF)C2)cc1F	0.055
714587	C[C@@H]1Cc2c([nH]c3ccc(F)cc23)[C@H](N1CC(F)(F)CO)c1c(F)cnc(OCCNCCCF)c1F	0.058
714482	COc1cnc(OCCNCCCF)cc1[C@H]1N(CC(F)(F)F)[C@H](C)Cc2c1[nH]c1ccccc21	0.059
50737190	C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@@H]2O)[C@H](CCCCCCCCCS(=O)CCCC(F)(F)C(F)(F)F)Cc1cc(O)ccc31	0.06
575904	COc1cc(OC2CN(CCCF)C2)ccc1[C@H]1N(CC(F)F)[C@H](C)Cc2c1ccc1[nH]ncc21	0.062
575898	COc1cc(NC2CN(CCCF)C2)ccc1[C@H]1N(CC(C)(F)F)[C@H](C)Cc2c1ccc1[nH]ncc21	0.063
714631	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CCC#N)c1c(F)ccc(OCCNCCCF)c1C	0.065
575916	COc1cc(NC2CN(CCCF)C2)ccc1[C@H]1N(CC(F)(F)F)[C@H](C)Cc2c1ccc1[nH]ncc21	0.065
727511	CC1=C([C@@H](Oc2ccc(O)cc12)c1ccc(OCCN2CC(CF)C2)cc1)c1cccc(O)c1	0.07
714679	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)CO)c1c(F)cnc(OCCNCCCF)c1Cl	0.07

714585	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)CO)c1c(F)cnc(OCCNCCCF)c1F	0.071
575958	C[C@@H]1Cc2c(ccc3[nH]ncc23)[C@H](N1CC(F)F)c1c(F)cc(NC2CN(CCCF)C2)cc1F	0.075
714581	C[C@@H]1Cc2c([nH]c3cccc(F)c23)[C@H](N1CC(F)(F)CO)c1c(F)ccc(OCCNCCCF)c1F	0.076
575870	C[C@@H]1Cc2c(ccc3[nH]ncc23)[C@H](N1CC(F)(F)CO)c1c(F)cc(NC2CN(CCCF)C2)cc1F	0.077
575956	C[C@@H]1Cc2c(ccc3[nH]ncc23)[C@H](N1CC(F)F)c1ccc(NC2CN(CCCF)C2)cc1	0.078
588294	COc1cc(OCCNCCCF)ncc1[C@H]1N(CC(C)(F)F)[C@H](C)Cc2c1[nH]c1ccccc21	0.079
588218	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(C)(C)F)c1c(F)cc(OCCNCCCF)cc1F	0.08
714524	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)F)c1c(F)ccc(OCCNCCCF)c1C	0.081
588310	COCC(C)(F)CN1[C@H](C)Cc2c([nH]c3ccccc23)[C@H]1c1c(F)cc(OCCNCCCF)cc1F	0.087
714476	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)F)c1c(F)ccc(OCCNCCCF)c1F	0.088
714627	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)CO)c1c(F)ccc(OCCNCCCF)c1Cl	0.089
50497452	CCCCCCCCCCCCNCCOc1ccc(cc1)C(=O)c1c(sc2cc(O)ccc12)-c1ccc(O)cc1	0.09
714486	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)CO)c1c(F)ccc(OCCNCCCF)c1F	0.092
588302	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)CO)c1c(F)cc(NCCNCCCF)cc1F	0.093
575882	C[C@@H]1Cc2c(ccc3[nH]ncc23)[C@H](N1CC1(F)CC1)c1c(F)cc(NC2CN(CCCF)C2)cc1F	0.094
714669	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)F)c1ccnc(OCCNCCCF)c1C	0.095
714593	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)CO)c1cccc(OCCNCCCF)c1C(F)F	0.095
575924	C[C@@H]1Cc2c(ccc3[nH]nc(F)c23)[C@H](N1CC(F)(F)F)c1ccc(NC2CN(CCCF)C2)cn1	0.096
575902	COc1cc(NC2CN(CCCF)C2)ccc1[C@H]1N(CC(F)F)[C@H](C)Cc2c1ccc1[nH]ncc21	0.098
714591	C[C@@H]1Cc2c([nH]c3ccc(F)cc23)[C@H](N1CC(F)(F)CO)c1c(F)cnc(OCCN(C)CCCF)c1F	0.099
575862	COCC(F)(F)CN1[C@H](C)Cc2c(ccc3[nH]ncc23)[C@H]1c1ccc(NC2CN(CCCF)C2)cc1OC	0.1
575886	COC[C@@](C)(F)CN1[C@H](C)Cc2c(ccc3[nH]ncc23)[C@H]1c1ccc(OC2CN(CCCF)C2)cc1OC	0.11
575932	C[C@@H]1Cc2c(ccc3[nH]ncc23)[C@H](N1CC(F)(F)F)c1ccc(NC2CN(CCCF)C2)cn1	0.12
714559	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)F)c1c(F)ccc(OCCNCCCF)c1F	0.12
714502	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)F)c1cc(OCCNCCCF)ccc1Cl	0.12
714613	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)F)c1c(Cl)ccc(OCCNCCCF)c1F	0.12
714577	C[C@@H]1Cc2c([nH]c3c(F)cccc23)[C@H](N1CC(F)(F)CO)c1c(F)ccc(OCCNCCCF)c1F	0.12
727515	C[C@@H](COc1ccc(cc1)[C@@H]1Oc2ccc(O)cc2C(C)=C1c1cccc(O)c1)N1CC[C@@H](C)C1	0.13
588318	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)F)c1c(F)cc(NCCNCCCF)cc1F	0.13
575982	C[C@@H]1Cc2c(ccc3[nH]nc(F)c23)[C@H](N1CC(F)(F)CO)c1ccc(NC2CN(CCCF)C2)cn1	0.13
575984	C[C@@H]1Cc2c(ccc3[nH]nc(F)c23)[C@H](N1CC(F)(F)CO)c1ccc(NC2CN(CCCF)C2)c(F)n1	0.13
50425039	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(C)(C)F)c1c(F)cc(\C=C\C(O)=O)cc1F	0.138038
714545	C[C@@H]1Cc2c([nH]c3ccccc23)[C@H](N1CC(F)(F)CO)c1cc(OCCNCCCF)ccc1Cl	0.14

Training Set **Test Set**